molecular dynamics model used in NASA's astrobiology research effort. The COSMOS code is often used to perform protein-folding simulations. Historically, many important problems involving 20,000-30,000 atoms have not scaled well on "clustered" parallel systems. This lack of performance is due to the small amount of work performed by each CPU relative to the time spent transferring data between CPUs.

The single-system approach of the SGI Origin 2000 architecture, and the large CPU count Lomax system in particular, offers an ideal platform for such computations. The Origin design supports very fast and low latency memory access times from any processor to any memory module. This low latency and high performance are essential for parallel scaling to the hundreds of CPUs necessary to execute problems in a timely manner.

The optimization effort is focused on inserting the highly efficient Ames-developed multi-level parallelism (MLP) approach into COSMOS. At this point the two major time-consuming routines have been converted with highly encouraging results. The first routine computes its zones between all water molecules in the system (WATNLS1). The second (MPFGATHER) gathers the forces for subsequent molecular movement. The results are summarized in Table 1.

Table 1. A comparison of COSMOS and COSMOS-MLP execution times.

COSMOS (32 CPUs)	COSMOS-MLP (343 CPUs)
Module Summary	Module Summary
WATNLS1: 56.66	WATNLS1: 0.94 (60x)
MPFGATHER: 42.13	MPFGATHER: 0.11 (383x)
BARRIER: 0.08	BARRIER: 1.97
Totals: 98.87	**Totals: 2.92 (36x)**

As the table shows, the MLP modifications dramatically improve the code performance on the two most time-dominating routines. The speedup arises from the much higher scaling efficiencies found in the MLP based parallel algorithm, coupled to a greater reuse of encached data. It is this expanded cache reuse that fuels the observed dramatic superlinear speedup over the old code executing at its parallel limit of 32 CPUs.

Current efforts indicate that COSMOS-MLP executions on Lomax will be some of the fastest ever achieved in this field. The results of this research have far-ranging implications in the commercial world, for the advanced numerical techniques developed under this effort are generally applicable to a number of industry standard models used by the university and drug research communities in the United States.

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Space Technology and CFD Applied to the Development of the DeBakey Heart Assist Device

Cetin Kiris, Dochan Kwak

Approximately 20 million people worldwide suffer annually from heart failure, a quarter of them in America alone. In the United States, only 2,500 donor hearts are available each year. The DeBakey Ventricular Assist Device (VAD) prolongs life until a suitable transplant heart is available, and is used to boost blood flow in patients suffering from hemodynamic deterioration, that is, loss of blood pressure and lowered cardiac output.

The use of computational fluid dynamics (CFD) technology led to major design improvements in the heart assist device, enabling its human implantation. The DeBakey VAD is a miniaturized heart pump designed to increase blood circulation in heart-failure patients awaiting a transplant. A ventricular assist device has to be small and efficient, generating a 5-liter-per-minute blood flow rate against

100 mm Hg pressure. Because blood is the operating fluid, the design of a VAD requires that it propel the blood gently, that is, it must minimize damage to the red blood cells. In order to reduce red blood cell damage, the pumping device must be designed to avoid regions of high shear stress and separated flow in the pump. In addition, the blood must be properly washed out of the pump since the formation of blood clots may appear within stagnation regions as a result of previously damaged blood cells. Since the device is small and the operating conditions severe, instrumentation for making necessary flow measurements is extremely difficult to design. Therefore it became necessary to look at the flow by computational means. The detailed computational flow analysis now affords VAD designers with a view of the complicated fluid dynamic processes inside their devices.

Through the collaborative efforts of MicroMed Technology Inc., Ames Research Center, and the Johnson Space Center, the device has evolved from early versions of the DeBakey VAD, which caused thrombus formation (blood clotting) and hemolysis (red blood cell damage). To solve these problems, Ames scientists employed shuttle main engine technology and CFD modeling capabilities, coupled with high-performance computing technology, to make several design modifications that vastly improved the VAD's performance. A three-dimensional, viscous, incompressible Navier–Stokes code (INS3D) was used to analyze the flow. Several design iterations were performed in order to increase the hydrodynamic performances of this axial pump. The research team investigated seven designs, altering cavity shapes, blade curvature, inlet cannula shapes, and impeller tip clearance size. They then suggested three major design modifications to solve the problems of cell damage resulting from their exposure to high shear stress and interrupted regions of blood flow in the DeBakey VAD (see figures 1 and 2).

The first improvement was the addition of an inducer that spins with the impeller, drawing the blood in and out of the device, thus preventing a back flow. Additionally, the inducer provides enough pressure rise to eliminate back flow in the impeller hub region. The front edges of the blades were slanted forward, allowing blood to flow at the correct angle with the impeller, thereby increasing the

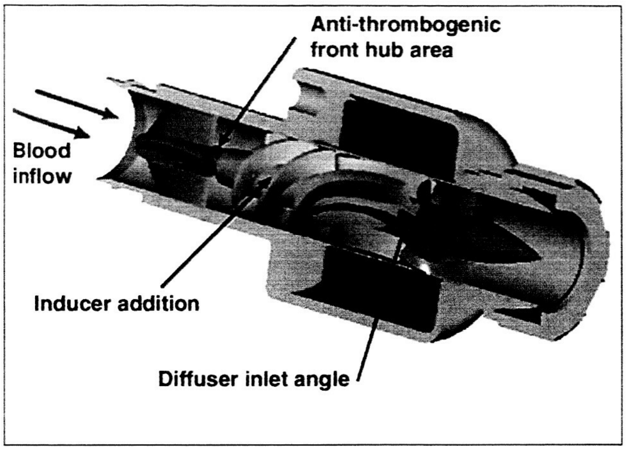

Fig. 1. Using CFD analysis, three major design modifications were made.

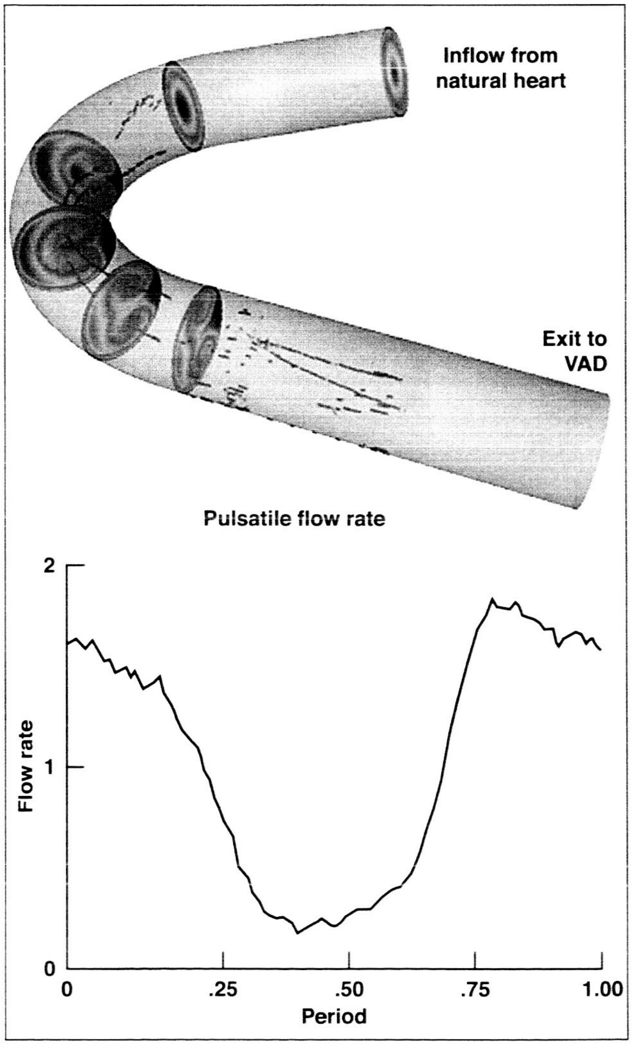

Fig. 2. Particle traces and velocity contours in the inlet cannula.

	Baseline design	New design
Hemolysis index	0.02	0.002
Thrombus formation	yes	no
Test run time	2 days	30+days

Fig. 3. Performance of the new VAD design.

efficiency of flow through the device. Second, CFD results suggested that the original design of the device caused clotting in the front bearing area where the blood passes over the flow straightener and meets the impeller blades. Expanding the hub area's width increased the circulation of blood, eliminating stagnant sections where clotting was known to occur. Additionally, researchers tapered the hub surface, accelerating blood flow, and thus creating good wall washing. And third, the exiting flow angle of the blood was examined and the diffuser angle was repositioned. Changing the diffuser blade angle aligns it with the blood flowing through the device, creating a smoother transition of blood over pump surfaces, and reducing the shear stress that causes cell damage.

Clinical tests conducted by MicroMed Technology and Baylor College of Medicine have confirmed the improvement in performance—hemolysis was decreased tenfold (figure 3). In collaboration with designers at MicroMed Technology, modifications made through the use of CFD analysis have resulted in a device that can perform for more than 100 days. The longest successful trial period to date in a human was 110 days, after which a donor heart was transplanted. The team's ultimate goal is to make the VAD a permanent alternative to heart transplant surgery. Successful European trials of the device in humans suggest its ability to provide long-term ventricular assistance.

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Application of Rotary-Wing Technologies to Planetary Science Missions

Larry A. Young

The next few years promise a unique convergence of NASA aeronautics and space programs. NASA planetary science missions are becoming increasingly more sophisticated and this will ultimately culminate, in part, in the development of planetary aerial vehicles (PAVs). Early work in this area has principally focused on conceptual design of fixed-wing aircraft configurations for Martian exploration. However, autonomous vertical-lift vehicles—and rotary-wing technologies in general—hold considerable potential for supporting planetary science and exploration missions.

For planetary science missions to Venus, Mars, and Titan, vertical-lift vehicles (using rotors as the means of propulsion) could potentially be developed and flown to support robotic science missions to these two planets and Saturn's moon (figure 1). For missions to Jupiter, Saturn, Uranus, and Neptune, vertical-lift capability is not required for PAVs supporting scientific investigations of the gas-giant planets. However, rotary-wing technologies, such as aeromechanics for PAV propeller design, could still be applicable for vehicles developed for these planets.

Autonomous vertical-lift PAVs would have the following advantages and capabilities when used for planetary exploration:

1. Their hover and low-speed flight capability would enable detailed and panoramic surveys of remote sites.
2. They would enable remote-site sample return to lander platforms or precision placement of scientific probes or both.
3. Soft landing capability would enable vehicle reuse (that is, lander refueling and multiple sorties) or remote-site monitoring and exploration.
4. Hover and soft landing provide good fail-safe "hold" modes for autonomous operation of PAVs.